Quantum Surface of Section Method: Decomposition of the Resolvent $(E - \hat{H})^{-1}$

Tomaž Prosen

Center for Applied Mathematics and Theoretical Physics,
University of Maribor, Krekova 2, SLO-62000 Maribor, Slovenia

Abstract The paper presents exact surface of section reduction of quantum mechanics. The main theoretical result is a decomposition of the energy-dependent propagator $\hat{G}(E) = (E - \hat{H})^{-1}$ in terms of the propagators which (also or exclusively) act in Hilbert space of complex-valued functions over the configurational surface of section, which has one dimension less than the original configuration space. These energy-dependent quantum propagators from and/or onto the configurational surface of section can be explicitly constructed as the solutions of the first order nonlinear Riccati-like initial value problems.

PACS numbers: 03.65.Db, 03.65.Ge, 02.30.+g, 05.45.+b

Submitted to **Zeitschrift für Physik B**

I. INTRODUCTION

In classical dynamics the concept of surface of section (SOS) was introduced by Poincaré and it has been proved to be very useful ever since [5]. Dynamics of the Hamiltonian system with f freedoms which is a smooth diffeomorphism in $2f$-dimensional phase space can be shown to be equivalent to discrete volume preserving mapping in $(2f-2)$-dimensional (sub-)phase space. Every trajectory (which is confined to $(2f-1)$-dim energy surface) typically crosses $(2f-2)$-dim intersection of $(2f-1)$-dim energy surface and $(2f-1)$-dim SOS infinitely many times (if the system is bound and the SOS is suitably chosen). The so called Poincaré map maps one such crossing to the next one and it is area (volume) preserving. Thus, for example, Hamiltonian systems of two freedoms can be reduced to area preserving maps of a 2-dim plane.

There were few attempts to extend a concept of SOS reduction to quantum mechanics but none have been completely successful yet. The quantum Poincaré map would be an energy-dependent propagator which would map (not yet firmly defined) amplitude distribution function over the $(f-1)$-dim projection of SOS to the configuration space to another. In bound systems, where no trajectory can escape, the quantum Poincaré map should become unitary in the semiclassical limit (It need not be unitary in nonsemiclassical regime). Bogomolny [1] proposes semiclassical propagator for the SOS map which is symmetric and approximately unitary (as $\hbar \to 0$). Bogomolny's map has a clear classical interpretation in terms of the classical trajectories, actions along them and corresponding monodromy matrices, but its greatest deficiency is that it is essentially semiclassical, so it cannot be viewed directly as an approximation of some exact quantum propagator. Smilansky, Doron and Schanz [2, 11] propose scattering approach for diagonalization of bound systems. Their method is almost exact (the error is of order $\mathcal{O}(\exp(-\mathrm{const}/\hbar))$ because they throw away the most of atenuating (evanescent) modes with imaginary wave number in order to make the basis for the S-matrix finite) but it is specialized for quantum billiards (Laplacians with Dirichlet boundary conditions). In fact for the billiards, Bogomolny's method is a limiting case (as $\hbar \to 0$) of the method of Smilansky and coworkers. Recently, Gutzwiller [4] published the exact quantum surface of section map for one system, namely, the free particle on a "trombone" attached to a parallelogram. My approach can be viewed as a generalization of the scattering approach to arbitrary quantum Hamiltonian system whose kinetic energy perpendicular to SOS is quadratic. Here I present a *local* version of the quantum surface of section method and prove its consistency in fairly rigorous manner. The central result is the proof of the decomposition formula for the energy-dependent Green's function in terms of energy-dependent propagators which act also (or exclusively, like my quantum Poincaré map) in the Hilbert space of functions over the configurational surface of section. Shortly after the present work had been completed I managed to develop a more straightforward *global* approach [7, 8] in terms of quantum mechanical scattering theory, although the present local theory gives some interesting results which were not obtained in [7, 8]. I have also applied the present method to calculate the eigenenergies with the sequential number around 20 million in a nonintegrable system, namely the so called *2-dim semi-separable oscillator* [9] which dynamically has all the generic features even though it is geometrically somewhat special. To the best of my knowledge this is the only available method enabling to calculate such high-lying eigenstates, which demonstrates not only the conceptual importance but also the practical power of the present method. After this work had been completed I have been informed

about a related work on the exact quantum SOS method of 2−dim Hamiltonians of the type $\boldsymbol{p}^2/2m + V(\boldsymbol{q})$ by Rouvinez and Smilansky [10].

In the Section II we will introduce convenient notation together with all the necessary definitions. Then the decomposition formula for the resolvent of the energy-dependent Green's function in terms of propagators which propagate from and/or onto the SOS will be presented and a comment on its interpretation will be given. In Section III the proof of the decomposition formula will be illustrated for the systems with single degree of freedom (1-dim configuration space). The proof of the general decomposition formula will be given in Section IV. Additional discussion on the interpretation of the quantum surface of section method and conclusions are found in section V.

II. DECOMPOSITION OF THE RESOLVENT

First I will introduce convenient notation for posing the problem. Vectors in f-dim configuration space manifold $\mathcal{C}$ (usually $\mathcal{C} = \Re^f$) will be denoted by $\boldsymbol{q}$ and vectors from the corresponding conjugate momentum space will be written as $\boldsymbol{p}$. The discussion will be limited only to the case where the SOS is perpendicular to the configuration space (CS), SOS $= \{(\boldsymbol{q}, \boldsymbol{p}); s(\boldsymbol{q}) = 0\}$. More general cases can generally be transformed to the upper one by the use of the canonical phase space transformations. Thus, we are considering only configurational surface of section $\mathcal{S}_0 = \{\boldsymbol{q} \in \mathcal{C}; s(\boldsymbol{q}) = 0\} \subset \mathcal{C}$. Assume that the topology of CS is simply connected and that function s can be globalized in a way that all members of the *family of surfaces of section* $\mathcal{S}_y = \{\boldsymbol{q} \in \mathcal{C}; s(\boldsymbol{q}) = y\}$ are topologically equivalent. Then the CS can be written as a Cartesian product $\mathcal{C} = \mathcal{S} \times [y_\downarrow, y_\uparrow]$, inducing the separation of coordinates $\boldsymbol{q} = (\boldsymbol{x}, y)$, $\boldsymbol{p} = (\boldsymbol{p}_x, p_y)$. Therefore one may write $\mathcal{S}_y = (\mathcal{S}, y)$. For the most useful example of Euclidean configuration space $\subseteq \Re^f$ with flat, mutually parallel surfaces of section this is already done by considering $(\boldsymbol{x}, y)$ as coordinates in Cartesian coordinate system where y-axis is oriented perpendicularly to SOS. The boundary surfaces $(\boldsymbol{x}, y_{\uparrow\downarrow})$ can be either at finite or infinite distance $y_{\uparrow\downarrow} \in \Re \cup \{-\infty, +\infty\}$. Every surface of section cuts the CS in two pieces which will be referred to as upper and lower and denoted by the value of the index $\sigma = \uparrow, \downarrow$. In arithmetic expressions, the arrows will have the following values, $\uparrow = +1, \downarrow = -1$. So, we will be considering not just one, but a whole family of surfaces of section at a time, where subvector $\boldsymbol{x}$ will denote the position inside SOS (parallel coordinates) and y will label the given SOS (perpendicular coordinate). This will be useful since it will turn out that the quantum SOS-SOS propagator (as will be defined below) for $\mathcal{S}_y$ uniquely determine such propagator for $\mathcal{S}_{y+dy}$ in nonlinear first order (Riccati-like) differential equation setting.

My theory presented in this paper will apply to quite general class of bound Hamiltonians (with possible generalizations to non-bound scattering problems) whose kinetic energy is quadratic at least perpendicularly to SOS

$$H = \frac{1}{2m} p_y^2 + H'(\boldsymbol{p}_x, \boldsymbol{x}, y). \tag{1}$$

The first term characterizes the perpendicular motion among surfaces of section and the second term captures the dynamics inside SOS. For some Hamiltonians which are not originally of this form this can be achieved by a proper choice of the SOS, i.e. the *coordinate system* $(\boldsymbol{x}, y)$. The parallel phase space coordinates $(\boldsymbol{x}, \boldsymbol{p}_{\boldsymbol{x}})$ may not be necessarily

of the Weyl-type but they may belong to arbitrary Lie group manifold as will become more clear when the theory will be developed (see discussion in section V).

In quantum mechanics, the observables are represented by self-adjoint operators in a Hilbert space $\mathcal{H}$ of complex-valued functions $\Psi(\boldsymbol{q})$ over the CS $\mathcal{C}$ which obey boundary conditions $\Psi(\boldsymbol{x}, y_{\uparrow\downarrow}) = 0$ and $\Psi(\boldsymbol{x} \in \partial\mathcal{S}$ or $|\boldsymbol{x}| \to \infty, y) = 0$ and have finite norm $\int_{\mathcal{C}} d\boldsymbol{q} |\Psi(\boldsymbol{q})|^2 < \infty$. We will use Dirac's notation. Pure state of a physical system can be represented by a vector — *ket* $|\Psi\rangle$ which can be expanded in a convenient complete set of basis vectors, e.g. position eigenvectors $|\boldsymbol{q}\rangle = |\boldsymbol{x}, y\rangle$, $|\Psi\rangle = \int_{\mathcal{C}} d\boldsymbol{q} |\boldsymbol{q}\rangle\langle\boldsymbol{q}|\Psi\rangle = \int_{\mathcal{C}} d\boldsymbol{q} \Psi(\boldsymbol{q})|\boldsymbol{q}\rangle$ (in a symbolic sense, since $|\boldsymbol{q}\rangle$ are not proper vectors, but such expansions are still meaningful iff $\Psi(\boldsymbol{q})$ is square integrable i.e. L^2-function). Every ket $|\Psi\rangle \in \mathcal{H}$ has a corresponding vector from the dual Hilbert space $\mathcal{H}'$, that is *bra* $\langle\Psi| \in \mathcal{H}'$, $\langle\Psi|\boldsymbol{q}\rangle = \langle\boldsymbol{q}|\Psi\rangle^*$. Now, fix a given SOS, $y = \text{const}$. Operators $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{p}}_{\boldsymbol{x}}$ can be viewed as acting on functions $\psi(\boldsymbol{x})$ of $\boldsymbol{x}$ only and therefore operating in some other, much smaller Hilbert space of square-integrable complex-valued functions over a given SOS $\mathcal{S}_y$. A family of such SOS-Hilbert spaces parametrized by y will be denoted by $\mathcal{L}_y$. Vectors in a SOS-Hilbert space $\mathcal{L}_y$ will be denoted by $|\psi\}_y$ (where subscript y will be omitted if possible). Eigenvectors of SOS position operators $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{x}}|\boldsymbol{x}'\} = \boldsymbol{x}'|\boldsymbol{x}'\}$ can provide a useful choice for the complete set of basis vectors of $\mathcal{L}_y$. $\{\boldsymbol{x}|\psi\} = \{\psi|\boldsymbol{x}\}^*$ can be interpreted as a quantum mechanical amplitude for a trajectory of a system being in quantum SOS-state $|\psi\}$ to cross SOS $\mathcal{S}_y$ at the point $\boldsymbol{x}$. Since surfaces $\mathcal{S}_y = (\mathcal{S}, y)$ are all topologically equivalent, the SOS-Hilbert spaces $\mathcal{L}_y$ are also all isomorphic, i.e. equivalent to some abstract SOS-Hilbert space $\mathcal{L}$. Isomorphism $\hat{I}_{y'y} \in Lin(\mathcal{L}_y, \mathcal{L}_{y'})$ (where $Lin(\mathcal{A}, \mathcal{B})$ denotes the set of all linear mappings from Hilbert space $\mathcal{A}$ to Hilbert space $\mathcal{B}$) is being provided by universal definition of the (symbolic) SOS-position eigenstates $|\boldsymbol{x}\}_y \equiv |\boldsymbol{x}\}$

$$\hat{I}_{y'y} = \int_{\mathcal{S}} d\boldsymbol{x}\, |\boldsymbol{x}\}_{y'}\, {}_y\{\boldsymbol{x}|, \tag{2}$$

which is the well known decomposition of identity of $\mathcal{L}_y$ for $y = y'$. The quantum Hamiltonian (like the classical one (1)) can be written as a sum of two terms

$$\hat{H} = -\frac{\hbar^2}{2m}\partial_y^2 + \hat{H}', \quad \hat{H}' = H'(\hat{\boldsymbol{p}}_x, \hat{\boldsymbol{x}}, \hat{y}) = H'(-i\hbar\partial_{\boldsymbol{x}}, \boldsymbol{x}, y), \tag{3}$$

where the eigenstates of the *inside Hamiltonian* $\hat{H}'$ restricted to the SOS-Hilbert space $\mathcal{L}_y$ (treating y as a parameter and not an operator), $|n\}_y \in \mathcal{L}_y$ called SOS-eigenmodes

$$\hat{H}'|_{\mathcal{L}_y}|n\}_y = E_n'(y)|n\}_y \tag{4}$$

provide very useful (countable $n = 1, 2, \ldots$) complete basis of $\mathcal{L}_y$ as will soon become clear.

Definition 1 *Let us define two families of Hilbert subspaces $\mathcal{H}^\sigma_{Ey_0} \subset \mathcal{H}, \sigma = \uparrow, \downarrow$ of L^2-functions which have definite energy, i.e. they satisfy Schrödinger equation, above/below a given SOS $\mathcal{S}_{y_0}$ and are zero below/above $\mathcal{S}_{y_0}$*

$$\mathcal{H}^\sigma_{Ey_0} = \{|\Psi\rangle \in \mathcal{H}; \quad \begin{array}{ll} \hat{H}\Psi(\boldsymbol{x}, y) = E\Psi(\boldsymbol{x}, y) & \text{if } \ \sigma y \geq \sigma y_0, \\ \Psi(\boldsymbol{x}, y) = 0, & \text{if } \ \sigma y < \sigma y_0\}. \end{array} \tag{5}$$

The values of $|\Psi\rangle \in \mathcal{H}^{\sigma}_{Ey_0}$ on the SOS $\mathcal{S}_{y_0}$, $\Psi(\boldsymbol{x}, y_0)$ are quite arbitrary [1] and represent a boundary condition for the time-independent Schrödinger equation which together with the remaining boundary condition $\Psi(\boldsymbol{x}, y_\sigma) = 0$ determines $|\Psi\rangle$ uniquely. This suggests that the spaces $\mathcal{L}_{y_0}$ and $\mathcal{H}^{\sigma}_{Ey_0}$ might be of the same size (elements of both are uniquely determined by the values of certain function on the $(f-1)$-dim SOS) and motivates the search for the connection between them. In order to achieve this we will use SOS-eigenmode (4) expansion of a state $|\Psi\rangle \in \mathcal{H}^{\sigma}_{Ey_0}$ near the surface $\mathcal{S}_{y_0}, y = y_0 + \sigma\epsilon, \epsilon \geq 0$,

$$\Psi(\boldsymbol{x}, y) = \sum_n \{\boldsymbol{x}|n\}_{y_0} \sqrt{\frac{-im}{\hbar^2 k_n(E, y_0)}} \left[c_n^{\text{out}} e^{i\sigma k_n(E,y_0)(y-y_0)} + c_n^{\text{onto}} e^{-i\sigma k_n(E,y_0)(y-y_0)}\right] + \mathcal{O}\left(\epsilon^2\right), \tag{6}$$

which is exact iff $\partial_y k_n(E, y) \equiv 0$, i.e. inside hamiltonian $\hat{H}'$ does not depend on the "parameter" y. Throughout this paper we will use the following definition of the complex square root $\sqrt{z} = \sqrt{\frac{1}{2}(|z| + \operatorname{Re} z)} + i\operatorname{sgn} \operatorname{Im} z \sqrt{\frac{1}{2}(|z| - \operatorname{Re} z)}$ which is a complex analytic function in upper half-plane $y \geq 0$. The accuracy of the ansatz (6) cannot be extended beyond the second order without extending the set of coefficients and differentiating quantities which depend on y_0, but this is quite enough, since the present form (6) correctly reproduces normal derivative $\partial_y \Psi(\boldsymbol{x}, y)$ and therefore also the probability currents through the SOS. The wavenumbers

$$k_n(E, y_0) = \sqrt{\frac{2m}{\hbar^2}(E - E_n(y_0))}, \tag{7}$$

which correspond to SOS-eigenmodes $|n\}_{y_0}$, assign the rest of the energy $E - E_n(y_0)$ to the perpendicular motion providing all terms in expansion (6) with the constant and correct value of the *effective* energy. The evanescent modes, for which $E_n(y_0) > E$, have imaginary wavenumbers. The coefficients $c_n^{\text{out}}, c_n^{\text{onto}}$ can be interpreted as the probability currents for SOS-eigenmodes to propagate out from the SOS and back onto the SOS, respectively. But only half of them are independent since the half of their nondegenerate linear combinations are arbitrary

$$c_n^{\text{out}} + c_n^{\text{onto}} = \sqrt{\frac{\hbar^2 k_n(E, y_0)}{-im}} \int_{\mathcal{S}} d\boldsymbol{x} \Psi(\boldsymbol{x}, y_0)\{n|\boldsymbol{x}\} \tag{8}$$

since boundary condition $\Psi(\boldsymbol{x}, y_0)$ is arbitrary and the other half of their linear combinations are fixed

$$c_n^{\text{out}} - c_n^{\text{onto}} = \sigma \sqrt{\frac{-i\hbar^2}{mk_n(E, y_0)}} \int_{\mathcal{S}} d\boldsymbol{x} \partial_y \Psi(\boldsymbol{x}, y_0)\{n|\boldsymbol{x}\} \tag{9}$$

since the normal derivative $\partial_y \Psi(\boldsymbol{x}, y_0)$ is determined by the solution of the Schrödinger equation $\hat{H}\Psi = E\Psi$ with boundary conditions $\Psi(\boldsymbol{x}, y_0)$ and $\Psi(\boldsymbol{x}, y_\sigma) = 0$. We choose the coefficients c_n^{out} to be arbitrary so the remaining coefficients c_n^{onto} are uniquely determined by c_n^{out}, and make the following definition.

[1] Of course, they should decay fast enough when $|\boldsymbol{x}| \to \infty$ in case when SOS is infinite.

Definition 2 *Take an arbitrary out-going quantum SOS-state* $|\psi^{\rm out}\}$ *with the eigenmode expansion* $|\psi^{\rm out}\} = \sum_n c_n^{\rm out}|n\}$*. Then the propagator from SOS back to SOS (above/below SOS if* $\sigma=\uparrow\downarrow$*, respectively) can be defined*

$$\hat{T}_\sigma(E, y_0) \in Lin(\mathcal{L}_{y_0}, \mathcal{L}_{y_0}) \tag{10}$$

and the on-going quantum SOS-state $|\psi^{\rm onto}\} = \sum_n c_n^{\rm onto}|n\}$ *can be written as*

$$|\psi^{\rm onto}\} = \hat{T}_\sigma(E, y_0)|\psi^{\rm out}\}. \tag{11}$$

Generally,

$$\hat{T}_\sigma(E, y_0) = \sum_{n,n'} c_n^{\rm onto}|_{(c_l^{\rm out}=\delta_{ln'})}|n\}\{n'|. \tag{12}$$

Let us join all the information about the SOS-eigenmodes (4) and their wavenumbers in the definition of the waveoperator $\hat{K}(E, y)$.

Definition 3 *Linear operator* $\hat{K}(E, y) \in Lin(\mathcal{L}_y)$ *is by definition an operator whose spectrum is just the set of wavenumbers* $\{k_n(E, y)\}$ *with SOS-eigenvectors* $|n\}_y$

$$\hat{K}(E, y) = \sum_n k_n(E, y)|n\}_y\, {}_y\{n| = \sqrt{\frac{2m}{\hbar^2}\left(E - \hat{H}'|_{\mathcal{L}_y}\right)}. \tag{13}$$

With aid of this new definition and the notation of Definition 2 one can write SOS-eigenmode expansion (6) more compactly [2]

$$\begin{aligned} \Psi(\boldsymbol{x}, y) &= \frac{\sqrt{-im}}{\hbar}\{\boldsymbol{x}|\hat{K}^{-1/2}(E, y_0)\left[e^{i\sigma\hat{K}(E,y_0)(y-y_0)} + e^{-i\sigma\hat{K}(E,y_0)(y-y_0)}\hat{T}_\sigma(E, y_0)\right]|\psi^{\rm out}\} \\ &+ \mathcal{O}\left(|y - y_0|^2\right) \end{aligned} \tag{14}$$

Lemma 1 *Expansion (14) holds for all states* $|\Psi\rangle$ *from all spaces* $\mathcal{H}^\sigma_{Ey_1}$*, such that* $\sigma y_1 \le \sigma y_0$*.*

The proof follows solely from the definition 1 of the spaces $\mathcal{H}^\sigma_{Ey}$, since all $\mathcal{H}^\sigma_{Ey_1}$ are equivalent on the domain $\{(\boldsymbol{x}, y); \boldsymbol{x} \in \mathcal{S}, \sigma y_0 \le \sigma y \le \sigma y_\sigma\}$, for $\sigma y_1 \le \sigma y_0$.

Definition 4 *Let* $\hat{P}_\sigma(E, y_0)$ *and* $\hat{Q}_\sigma(E, y_0)$ *be the quantum propagators from upper/lower (*$\sigma=\uparrow\downarrow$*) part of CS* $\mathcal{C}$ *to SOS* $\mathcal{S}_{y_0}$ *and vice-versa*

$$\hat{Q}_\sigma(E, y_0) \in Lin(\mathcal{L}_{y_0}, \mathcal{H}) \tag{15}$$

$$\hat{P}_\sigma(E, y_0) \in Lin(\mathcal{H}, \mathcal{L}_{y_0}) \tag{16}$$

[2] The SOS-SOS propagator $\hat{T}_\sigma(E, y_0)$ can be viewed also as a scattering operator of the following scattering problem which is obtained from the orginal bound Hamiltonian $\hat{p}_y^2/2m + H'(\hat{p}_{\boldsymbol{x}}, \boldsymbol{x}, y)$ by substituting it in one part of CS, $\sigma y \le \sigma y_0$, by the $y-$flat waveguide with the Hamiltonian $\hat{p}_y^2/2m + H'(\hat{p}_{\boldsymbol{x}}, \boldsymbol{x}, y_0)$, for $\sigma y \le \sigma y_0$.

such that for arbitrary states $|\psi^{\rm out}\} \in \mathcal{L}_{y_0}, \{\psi^{\rm onto}| \in \mathcal{L}'_{y_0}$

$$\hat{Q}_\sigma(E,y_0)|\psi^{\rm out}\} \in \mathcal{H}^\sigma_{Ey_0} \tag{17}$$
$$\{\psi^{\rm onto}|\hat{P}_\sigma(E,y_0) \in \mathcal{H}^{\sigma\prime}_{E^*y_0} \tag{18}$$

which are uniquely determined by the boundary condition on the SOS $\mathcal{S}_{y_0}$

$$\langle \boldsymbol{x}, y_0|\hat{Q}_\sigma(E,y_0)|\psi^{\rm out}\} = \frac{\sqrt{-im}}{\hbar}\{\boldsymbol{x}|\hat{K}^{-1/2}(E,y_0)(1+\hat{T}_\sigma(E,y_0))|\psi^{\rm out}\} \tag{19}$$
$$\{\psi^{\rm onto}|\hat{P}_\sigma(E,y_0)|\boldsymbol{x},y_0\rangle = \frac{\sqrt{-im}}{\hbar}\{\psi^{\rm onto}|(1+\hat{T}_\sigma(E,y_0))\hat{K}^{-1/2}(E,y_0)|\boldsymbol{x}\} \tag{20}$$

Here, perhaps, a remark is in order: Conjugated energy E^* was used in (18) in order to make propagator $\hat{P}_\sigma(E,y)$ complex analytic function of E rather than E^*.

Now all the necessary tools are prepared to state the main result of this paper:

Theorem 1 *The energy-dependent quantum propagator (i.e. the resolvent of the Hamiltonian)* $\hat{G}(E) = (E-\hat{H})^{-1}$ *can be decomposed in terms of the CS-CS propagator — with* no intersection with the *SOS* $\mathcal{S}_y$ — $\hat{G}_0(E,y)$*, CS-SOS propagator* $\hat{P}_\sigma(E,y)$*, SOS-CS propagator* $\hat{Q}_\sigma(E,y)$*, and SOS-SOS propagator* $\hat{T}_\sigma(E,y)$

$$\begin{aligned}\hat{G}(E) = \hat{G}_0(E,y) &+ \sum_\sigma \hat{Q}_\sigma(E,y)(1-\hat{T}_{-\sigma}(E,y)\hat{T}_\sigma(E,y))^{-1}\hat{P}_{-\sigma}(E,y) \\ &+ \sum_\sigma \hat{Q}_\sigma(E,y)(1-\hat{T}_{-\sigma}(E,y)\hat{T}_\sigma(E,y))^{-1}\hat{T}_{-\sigma}(E,y)\hat{P}_\sigma(E,y),\end{aligned} \tag{21}$$

and all poles of the Green's function $\hat{G}(E)$ *are in one-to-one correspondence with the singularities of* $(1-\hat{T}_\sigma(E,y)\hat{T}_{-\sigma}(E,y))^{-1}$ *where the four propagators* $\hat{P}_\sigma(E,y), \hat{Q}_\sigma(E,y), \hat{T}_\sigma(E,y)$*, and* $\hat{G}_0(E,y)$ *are analytic.* [3]

The propagator $\hat{G}_0(E,y)$ can be calculated from (21) if the Green's function $\hat{G}(E)$ is known explicitly, but it is less important, since its contribution becomes negligible when the energy E approaches an eigenenergy (pole). Note that $\langle \boldsymbol{q}'|\hat{G}_0(E,y)|\boldsymbol{q}\rangle$ is the probability amplitude to propagate from point $\boldsymbol{q}$ to point $\boldsymbol{q}'$ at energy E and without hitting the SOS $\mathcal{S}_y$ in between, so it is equal to zero if initial and final point, $\boldsymbol{q}$ and $\boldsymbol{q}'$, lie on different sides of the SOS $\mathcal{S}_y$. The decomposition formula (21) has a very strong physical interpretation. In order to see this most clearly we omit the arguments (E,y) and formally expand $(1-\hat{T}_\sigma\hat{T}_{-\sigma})^{-1}$ in terms of the geometric series

$$\begin{aligned}\hat{G} = \hat{G}_0 &+ \hat{Q}_\downarrow\hat{P}_\uparrow + \hat{Q}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{P}_\uparrow + \hat{Q}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{P}_\uparrow + \ldots \\ &+ \hat{Q}_\uparrow\hat{P}_\downarrow + \hat{Q}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{P}_\downarrow + \hat{Q}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{P}_\downarrow + \ldots \\ &+ \hat{Q}_\uparrow\hat{T}_\downarrow\hat{P}_\uparrow + \hat{Q}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{P}_\uparrow + \hat{Q}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{P}_\uparrow + \ldots \\ &+ \hat{Q}_\downarrow\hat{T}_\uparrow\hat{P}_\downarrow + \hat{Q}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{P}_\downarrow + \hat{Q}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{T}_\uparrow\hat{P}_\downarrow + \ldots\end{aligned} \tag{22}$$

The arguments (E,y) will also be omitted to increase transparency in the rest of this paper whenever this will cause absolutely no confusion. The meaning of this expression (22)

[3]The latter propagators are non-analytic e.g. at thresholds for opening of new modes E'_n where $k_n(E'_n,y) = 0$.

when put in a sandwich between $\langle \boldsymbol{q}'|$ and $|\boldsymbol{q}\rangle$ is that the *probability amplitude to propagate from point* $\boldsymbol{q}$ *to* $\boldsymbol{q}'$ *at energy* E (PAPPE) is a sum of: (i) PAPPE without hitting the SOS ($\hat{G}_0$ term) plus (ii) PAPPE with single intersection with SOS ($\hat{Q}\hat{P}$ terms) plus (iii) PAPPE with double intersection with SOS ($\hat{Q}\hat{T}\hat{P}$ terms) plus ... The alternating symbols $\uparrow\downarrow$ in a compositum like $\hat{Q}_\downarrow\hat{T}_\uparrow\hat{T}_\downarrow\hat{P}_\uparrow$ (see Figure 1) mean that the system should be on different sides of the SOS before and after it crosses the SOS, since typical quantum trajectory (in the sense of summing over paths) is continuous. The proof of the statements made in this section will be given in Section IV. A more lengthy discussion on the interpretation can be found in section V.

III. ONE-DIMENSIONAL CASE

First we shall prove the Theorem 1 for the special case of systems with a one degree of freedom $f = 1$. Thus the main idea of the proof will be more transparent and the reader will follow the next section, which is a natural continuation of the previous one, more easily. Ozorio de Almeida [6] published a similar study of one-dimensional systems in the context of exact quantum SOS method for *separable systems*.

Now the configuration space is just the interval (or the whole real axis) $\mathcal{C} = [y_\downarrow, y_\uparrow]$ and the surfaces of section $\mathcal{S}_{y_0}$ are single points $y = y_0$. Thus the SOS-Hilbert spaces $\mathcal{L}_{y_0}$ are one-dimensional with one normalized basis vector $|1\}$ and the SOS-SOS propagator is just a simple complex-valued function $T_\sigma(E, y_0) = \{1|\hat{T}_\sigma(E, y_0)|1\}$ which can be also represented with the phase shift $\delta_\sigma(E, y_0)$ between the outgoing and the incoming wave in the local expansion (analogous to (6,14)) of the (real) wavefunction $|\Psi^\sigma_{Ey_0}\rangle \in \mathcal{H}^\sigma_{Ey_0}$

$$\Psi^\sigma_{Ey_0}(y) = \sqrt{\frac{4m}{\hbar^2 k(E, y_0)}} \cos\left(k(E, y_0)(y - y_0) + \tfrac{1}{2}\delta_\sigma(E, y_0)\right) + \mathcal{O}\left(\epsilon^2\right), \tag{23}$$

$$T_\sigma(E, y_0) = e^{-i\sigma\delta_\sigma(E, y_0)}, \tag{24}$$

where $y = y_0 + \sigma\epsilon$, $\epsilon \geq 0$. The propagators onto/from the SOS $P_\sigma(E, y_0, y) = \{1|\hat{P}_\sigma(E, y_0)|y\rangle$ and $Q_\sigma(E, y, y_0) = \langle y|\hat{Q}_\sigma(E, y_0)|1\}$ are now unique solutions of the Schrödinger equations

$$\begin{array}{l}(\partial_y^2 + k^2(E, y))P_\sigma(E, y_0, y) = 0 \\ (\partial_y^2 + k^2(E, y))Q_\sigma(E, y, y_0) = 0\end{array} \qquad k^2(E, y) = \frac{2m}{\hbar^2}(E - V(y)) \tag{25}$$

with boundary conditions

$$Q_\sigma(E, y_0, y_0) = P_\sigma(E, y_0, y_0) = \sqrt{\frac{-4im}{\hbar^2 k(E, y_0)}} \cos\left(\tfrac{1}{2}\delta_\sigma(E, y_0)\right) e^{-i\sigma\frac{1}{2}\delta_\sigma(E, y_0)} \tag{26}$$

$$Q_\sigma(E, y_\sigma, y_0) = P_\sigma(E, y_0, y_\sigma) = 0. \tag{27}$$

It is convenient to express the SOS-CS-SOS propagators in terms of the standardized (real) solution of the Schrödinger equation

$$Q_\sigma(E, y_0, y) = P_\sigma(E, y, y_0) = \Psi^\sigma_{Ey_0}(y) e^{-i\sigma\frac{1}{2}\delta(E, y_0) - i\frac{\pi}{4}}. \tag{28}$$

Let the matrix elements of the Green's functions be denoted by $G(E, y', y) = \langle y'|\hat{G}(E)|y\rangle$, $G_0(E, y_0, y', y) = \langle y'|\hat{G}_0(E, y_0)|y\rangle$. The decomposition formula in one dimension can now

be written as

$$
\begin{aligned}
G(E,y',y) &= G_0(E,y_0,y',y)+\\
&+ Q_\downarrow(E,y',y_0)(1-T_\uparrow T_\downarrow)^{-1}P_\uparrow(E,y_0,y)+\\
&+ Q_\uparrow(E,y',y_0)(1-T_\downarrow T_\uparrow)^{-1}P_\downarrow(E,y_0,y)+\\
&+ Q_\uparrow(E,y',y_0)(1-T_\downarrow T_\uparrow)^{-1}T_\downarrow P_\uparrow(E,y_0,y)+\\
&+ Q_\downarrow(E,y',y_0)(1-T_\uparrow T_\downarrow)^{-1}T_\uparrow P_\downarrow(E,y_0,y)= \qquad (29)\\
&= G_0(E,y',y)-\frac{\sum_\sigma\left(\Psi^\sigma_{Ey_0}(y')\Psi^{-\sigma}_{Ey_0}(y)+\Psi^\sigma_{Ey_0}(y')\Psi^\sigma_{Ey_0}(y)e^{-i\frac{1}{2}\delta}\right)}{2\sin\left(\frac{1}{2}\delta\right)} \qquad (30)
\end{aligned}
$$

where $\delta=\delta_\uparrow(E,y_0)-\delta_\downarrow(E,y_0)$. There are then two points to be proved:

- **Point 1** All the poles of the Green function $G(E,y',y)$ in complex energy E plane should come from singularities of $(1-T_\uparrow(E,y_0)T_\downarrow(E,y_0))^{-1}$ and vice versa.
- **Point 2** The residuum of the decomposed Green function $G(E,y',y)$ at the pole — eigenenergy E_0 should be equal to $\Psi(y)\Psi(y')$ where $\Psi(y)$ is a *normalized* real eigenfunction at energy E_0 provided that all the propagators G_0, P_σ, Q_σ and T_σ are analytic at E_0.

The first point is easy. The RHS of (29,30) has a singularity if $T_\uparrow(E,y_0)T_\downarrow(E,y_0)=1$. i.e.

$$\delta_\uparrow(E,y_0)-\delta_\downarrow(E,y_0)=0 \pmod{2\pi}. \qquad (31)$$

This happens if and only if E is an eigenvalue of the Schrödinger operator $\hat{H}$ since the two partial solutions of the Schrödinger equation $\Psi^\sigma_{Ey_0}(y)$, $\sigma=\uparrow,\downarrow$ (see equation (23)) can be joined into the continuous and differentiable (at SOS $y=y_0$) eigenfunction

$$\frac{\partial_y\Psi^\uparrow_{Ey_0}(y_0)}{\Psi^\uparrow_{Ey_0}(y_0)}=\frac{\partial_y\Psi^\downarrow_{Ey_0}(y_0)}{\Psi^\downarrow_{Ey_0}(y_0)}, \qquad (32)$$

but $\Psi^\uparrow_{Ey_0}(y_0)=(\cos\delta_\downarrow/\cos\delta_\uparrow=\pm1)\Psi^\downarrow_{Ey_0}(y_0)$. The quantization condition (31,32) is independent of the position of the SOS $y=y_0$, although in classically forbidden regions where the wavenumber is imaginary $k^2(E,y_0)<0$ the phase-shift $\delta_\sigma(E,y_0)$ is also imaginary number (plus an integer multiple of π) and the SOS-SOS propagator $T_\sigma(E,y_0)$ becomes real with the magnitude which is different from unity.

The second point is more elaborate. Let us define a global solution of the Schrödinger equation $|\Psi_{Ey_0}\rangle\in\mathcal{H}$

$$|\Psi_{Ey_0}\rangle=|\Psi^\uparrow_{Ey_0}\rangle\pm|\Psi^\downarrow_{Ey_0}\rangle \qquad (33)$$

where we chose the sign ($\pm$ if $\frac{1}{2}\delta$ is an even/odd multiple of π) in order to make the eigenfunction $\Psi_{E_0y_0}(y)$ continuous at the SOS y_0. In the position representation $\Psi_{Ey_0}(\boldsymbol{x},y)=\Psi^\uparrow_{Ey_0}(\boldsymbol{x},y)\pm\Psi^\downarrow_{Ey_0}(\boldsymbol{x},y)$, one term is always zero and the other is not. If E_0 is an eigenenergy which satisfies quantization condition (31) then the residuum of (30) is

$$\operatorname*{Res}_{E=E_0} G(E,y',y)=-\frac{\Psi_{E_0y_0}(y')\Psi_{E_0y_0}(y)}{\partial_E\delta_\uparrow(E_0,y_0)-\partial_E\delta_\downarrow(E_0,y_0)}. \qquad (34)$$

In order to calculate the energy derivative of the phase shift $\partial_E \delta_\sigma(E,y)$ we should first study its dependence on y. Note that any wavefunction $\Psi(y)$ which satisfies the Schrödinger equation

$$(\partial_y^2 + k^2(E,y))\Psi(y) = 0, \quad \text{with} \quad \Psi(y_\sigma) = 0 \tag{35}$$

is proportional to $\Psi^\sigma_{Ey_0}(y)$, for $\sigma y \geq \sigma y_0$ (see lemma 1)

$$\Psi(y) = a\cos\left(k(E,y_0)(y-y_0) + \tfrac{1}{2}\delta_\sigma(E,y_0)\right) + \mathcal{O}\left(|y-y_0|^2\right). \tag{36}$$

Let us differentiate this equation with respect to y, then set $y_0 = y$ and substitute $\Psi(y)$ back, giving

$$\partial_y \Psi(y) = -k(E,y)\tan\left(\tfrac{1}{2}\delta(E,y)\right)\Psi(y) \tag{37}$$

Now, differentiate the equation (37) with respect to y, use Schrödinger equation on the LHS and again (37) on the RHS. After cancelling the $\Psi(y)$ on both sides one obtains closed first order nonlinear differential equation for the phase-shifts

$$\partial_y \delta = 2k - \frac{\partial_y k}{k}\sin(\delta), \tag{38}$$

which is equivalent to the Riccati equation for the propagator T_σ

$$\partial_y T_\sigma = -2i\sigma k T_\sigma + \frac{\partial_y k}{2k}(1 - T_\sigma^2). \tag{39}$$

The corresponding *initial* conditions are

$$\begin{array}{lll} \delta_\sigma(E,y_\sigma) = \pi, & T_\sigma(E,y_\sigma) = -1 & \text{if } \; k^2(E,y_\sigma) \geq 0, \\ \delta_\sigma(E,y_\sigma) = n\pi - i\sigma\infty, & T_\sigma(E,y_\sigma) = 0 & \text{if } \; k^2(E,y_\sigma) < 0. \end{array} \tag{40}$$

Then we define the so-called *incomplete normalization constants* $N_\sigma(E,y)$

$$N_\sigma(E,y_0) = \int_{y_0}^{y_\sigma} dy \left[\Psi^\sigma_{Ey_0}(y)\right]^2. \tag{41}$$

Again we shall investigate the $y-$dependence of incomplete normalization constants. Since $\Psi_{Ey_0}(y)$ is again proportional to some arbitrary wavefunction $\Psi(x)$ satisfying Schrödinger *initial value problem* (35) (lemma 1) we can write

$$\Psi^\sigma_{Ey_0}(y) = \Psi^\sigma_{Ey_0}(y_0)\frac{\Psi(y)}{\Psi(y_0)}. \tag{42}$$

Use a substitution (42) in the definition of $N_\sigma(E,y_0)$ (41), then move everything that does not depend on the integration variable y to the LHS and derive with respect to y_0, giving

$$\partial_{y_0}\left[\frac{\hbar^2 k(E,y_0)\Psi^2(y_0)}{4m\cos^2\left(\frac{1}{2}\delta_\sigma(E,y_0)\right)}N_\sigma(E,y_0)\right] = -\Psi^2(y_0)$$

After performing the differentiation and using the formulas (37) and (38) for the derivative of $\Psi(y)$ and $\delta_\sigma(E,y)$ with respect to y one obtains a first order differential equation for the incomplete normalization constants

$$\partial_y N_\sigma + \frac{\partial_y k}{k}\cos(\delta_\sigma)N_\sigma = -\frac{2m}{\hbar^2 k}(1 + \cos(\delta_\sigma)), \tag{43}$$

$$N_\sigma(E,y_\sigma) = 0. \tag{44}$$

Armed with formulas (38,43) we are ready to determine the energy derivative of the phase-shift $\partial_E \delta_\sigma(E, y)$ which is most valuable to us. It can be uniquely determined from the differential equation which expresses the uniqueness of the mixed second derivative

$$\partial_y(\partial_E \delta_\sigma) = \partial_E(\partial_y \delta_\sigma) \tag{45}$$

since the initial conditions are also known

$$\partial_E \delta_\sigma(E, y_\sigma) = 0. \tag{46}$$

The author has used a heuristic ansatz

$$\partial_E \delta_\sigma = -N_\sigma + u(E, y)\cos(\delta_\sigma) + v(E, y)\sin(\delta_\sigma) \tag{47}$$

and found that it is consistent with the system (45,46) iff $u = 0$ and $v = -\frac{m}{\hbar^2 k^2}$, so

$$\partial_E \delta_\sigma = -N_\sigma - \frac{m}{\hbar^2 k^2}\sin(\delta_\sigma). \tag{48}$$

Now, we can easily prove the rest of the decomposition formula with the calculation of the residuum (34). If E_0 is an eigenenergy then from the quantization condition (31) one has $\sin(\delta_\uparrow(E_0, y_0)) = \sin(\delta_\downarrow(E_0, y_0))$ and so the denominator of (34)

$$\begin{aligned} &\partial_E \delta_\uparrow(E_0, y_0) - \partial_E \delta_\downarrow(E_0, y_0) = -(N_\uparrow(E_0, y_0) - N_\downarrow(E_0, y_0)) = \\ &= -N(E_0, y_0) = -\int_{y_\downarrow}^{y_\uparrow} dy\, [\Psi_{E_0 y_0}(y)]^2 \end{aligned} \tag{49}$$

is just a negative *(complete) normalization constant* which makes the residuum equal to the product of normalized eigenfunctions

$$\operatorname*{Res}_{E=E_0} G(E, y', y) = \Psi(y)\Psi(y'), \quad \Psi(y) = \frac{\Psi_{E_0 y_0}(y)}{\sqrt{N(E_0, y_0)}}. \tag{50}$$

q.e.d.

IV. PROOF OF THE GENERAL CASE

To prove the general decomposition formula (21) of Theorem 1 we shall use roughly the same procedure as for the 1-dim case in previous section although few steps will be more lengthy now.

First we have to prove (see Point 1, Section III) that all poles of the Green's operator (resolvent) $\hat{G}(E)$ are due to singularities of $(1 - \hat{T}_\downarrow(E, y_0)\hat{T}_\uparrow(E, y_0))$ in the energy region where the propagator $\hat{T}_\sigma(E, y_0)$ is well defined. The threshold energies for opening of new modes $E'_n(y_0)$ should be excluded so that the inverse $\hat{K}^{-1/2}(E, y_0)$ which enters into the definition of $\hat{T}_\sigma(E, y_0)$ is well defined.

Any wavefunction $\Psi^\sigma_{Ey_0}(\boldsymbol{x}, y)$ which satisfies Schrödinger equation above/below y_0, $|\Psi^\sigma_{Ey_0}\rangle \in \mathcal{H}^\sigma_{Ey_0}$ can be represented with some $|\psi\} \in \mathcal{L}_{y_0}$ in a form

$$\Psi^\sigma_{Ey_0}(\boldsymbol{x}, y) = \langle \boldsymbol{x}, y|\hat{Q}_\sigma(E, y_0)|\psi\}. \tag{51}$$

If E_0 is such a pole, i.e. an eigenenergy of the Hamiltonian $\hat{H}$, then the corresponding eigenfunction $\Psi_1(\boldsymbol{x}, y)$ and its normal derivative $\partial_y \Psi_1(\boldsymbol{x}, y)$ should be continuous on the SOS $\mathcal{S}_{y_0}$. In general, the eigenenergy E_0 can sometimes be degenerate, i.e. the corresponding eigenspace can be more than one, say, d-dimensional spanned by the eigenfunctions $\Psi_n(\boldsymbol{x}, y), n = 1 \ldots d$. So, there should exist $2d$ SOS-states $|\sigma n\} \in \mathcal{L}_{y_0}$, $n = 1 \ldots d$, $\sigma = \uparrow, \downarrow$ such that

$$\Psi_n(\boldsymbol{x}, y) = \begin{cases} \langle \boldsymbol{x}, y|\hat{Q}_\uparrow(E_0, y_0)| \uparrow n\} & \text{if } \; y \geq y_0, \\ \langle \boldsymbol{x}, y|\hat{Q}_\downarrow(E_0, y_0)| \downarrow n\} & \text{if } \; y < y_0, \end{cases} \tag{52}$$

with

$$\begin{aligned} \langle \boldsymbol{x}, y_0|\hat{Q}_\uparrow(E_0, y_0)| \uparrow n\} &= \langle \boldsymbol{x}, y_0|\hat{Q}_\downarrow(E_0, y_0)| \downarrow n\} \\ \partial_y \langle \boldsymbol{x}, y|\hat{Q}_\uparrow(E_0, y_0)| \uparrow n\}|_{y \searrow y_0} &= \partial_y \langle \boldsymbol{x}, y|\hat{Q}_\downarrow(E_0, y_0)| \downarrow n\}|_{y \nearrow y_0}. \end{aligned} \tag{53}$$

Continuity relations (53) can be rewritten by using expansion (14) to calculate the normal derivative

$$\partial_y \langle \boldsymbol{x}, y|\hat{Q}_\sigma(E, y_0)|\psi\}|_{\sigma y \searrow \sigma y_0} = \sigma \frac{\sqrt{im}}{\hbar} \{\boldsymbol{x}|\hat{K}^{1/2}(E, y_0) \left(1 - \hat{T}_\sigma(E, y_0)\right) |\psi\} \tag{54}$$

and by using the completeness of position SOS-states $|\boldsymbol{x}\}$,

$$\left(1 + \hat{T}_\uparrow(E_0, y_0)\right) | \uparrow n\} = \left(1 + \hat{T}_\downarrow(E_0, y_0)\right) | \downarrow n\}, \tag{55}$$

$$\left(1 - \hat{T}_\uparrow(E_0, y_0)\right) | \uparrow n\} = -\left(1 - \hat{T}_\downarrow(E_0, y_0)\right) | \downarrow n\}. \tag{56}$$

Adding and subtracting equations (55,56) one obtains important relations

$$\hat{T}_\sigma(E_0, y_0)|\sigma n\} = | - \sigma n\}, \tag{57}$$

which mean that the operator $1 - \hat{T}_{-\sigma}(E_0, y_0)\hat{T}_\sigma(E_0, y_0)$ is singular with $|\sigma n\}$ being the corresponding right null-vectors

$$\left(1 - \hat{T}_{-\sigma}(E_0, y_0)\hat{T}_\sigma(E_0, y_0)\right) |\sigma n\} = 0. \tag{58}$$

By deriving the SOS-quantization condition (58) we have proved the point 1 completely, since the reasoning (52-58) can easily be reversed: existence of d-dim nulspace of operator $1 - \hat{T}_{-\sigma}(E_0, y_0)\hat{T}_\sigma(E_0, y_0)$ implies the existence of d-dim eigenspace of the Hamiltonian $\hat{H}$. Each d SOS-states $|\sigma n\}, n = 1 \ldots d$ are linearly independent, since $\sum_n c_n |\sigma n\} = 0$ would imply $\sum_n c_n |\Psi_n\rangle = 0$ due to linearity of relation (52). The null-space of $1 - \hat{T}_{-\sigma}(E_0, y_0)\hat{T}_\sigma(E_0, y_0)$ which is spanned by $|\sigma n\}$, $n = 1 \ldots n$ is therefore also d-dimensional. [4] We shall soon need also the *complementary* SOS-representation of the (complex conjugated) eigenfunctions $\Psi_n^*(\boldsymbol{x}, y)$ which are in analogy with (52) provided by propagators $\hat{P}_\sigma(E_0, y_0)$. There exists $2d$ SOS-states $|\sigma n^*\} \in \mathcal{L}_{y_0}$, $n = 1 \ldots d$, $\sigma = \uparrow, \downarrow$, such that

$$\Psi_n^*(\boldsymbol{x}, y) = \begin{cases} \{\uparrow n^*|\hat{P}_\uparrow(E_0, y_0)|\boldsymbol{x}, y\rangle & \text{if } \; y \geq y_0, \\ \{\downarrow n^*|\hat{P}_\downarrow(E_0, y_0)|\boldsymbol{x}, y\rangle & \text{if } \; y < y_0. \end{cases} \tag{59}$$

Requiring continuity of eigenfunctions and their normal derivatives results in a sequence of formulas completely analogous to (53-56) ending with

$$\{\sigma n^*|\hat{T}_\sigma(E_0, y_0) = \{-\sigma n^*|, \tag{60}$$

[4] This is another proof of the Sturm-Liouville theorem which forbids degeneracies in one dimension since then SOS-Hilbert space $\mathcal{L}$ is 1-dimensional, and so d cannot be greater than 1.

and the complementary quantization condition

$$\{-\sigma n^*| \left(1 - \hat{T}_{-\sigma}(E_0, y_0)\hat{T}_\sigma(E_0, y_0)\right) = 0. \tag{61}$$

We have still to prove (see Point 2, Section III) that the residuum of the energy dependent Green's function $\mathrm{Res}_{E=E_0}\langle \boldsymbol{q}'|\hat{G}(E)|\boldsymbol{q}\rangle$ is equal to the sum (in case of degeneracy) of products of orthonormalized eigenfunctions $\sum_{n=1}^{d} \Psi_n(\boldsymbol{q}')\Psi_n^*(\boldsymbol{q})$ where complex conjugation should be used carefully since eigenfunctions are no longer necessarily real. So let us assume that our sample functions which span the eigenspace at E_0 are orthonormal $\langle \Psi_n|\Psi_l\rangle = \delta_{nl}$. The following lemma will be found very useful for calculating the residui of operator-valued functions.

Lemma 2 *Let $\hat{A}$ be a singular operator $\hat{A} \in Lin(\mathcal{L})$ with $d-$dimensional left and right null-space. If $|L_n\}, |R_n\} \in \mathcal{L}$, $n = 1 \ldots d$ span the left and right null space $\mathcal{N}_L = \ker(\hat{A}^\dagger)$ and $\mathcal{N}_R = \ker(\hat{A})$, respectively, then*

$$\operatorname*{Res}_{z=0}(z - \hat{A})^{-1} = \sum_{n,l=1}^{d} Inv_{nl}[\{L_n|R_l\}]|R_n\}\{L_l| \tag{62}$$

where $Inv_{nl}[c_{nl}]$ denotes the finite-dimensional-matrix inversion,

$$\sum_{l=1}^{d} Inv_{nl}[\{L_n|R_l\}]\{L_l|R_{n'}\} = \sum_{l=1}^{d}\{L_n|R_l\}Inv_{ln'}[\{L_l|R_{n'}\}] = \delta_{nn'} \tag{63}$$

Proof Let the left and right images be denoted by $\mathcal{I}_L = \hat{A}^\dagger\mathcal{L}$ and $\mathcal{I}_R = \hat{A}\mathcal{L}$, respectively. We note that,

$$\begin{aligned} \mathcal{I}_R &= \mathcal{N}_L^\perp, & (64)\\ \mathcal{I}_L &= \mathcal{N}_R^\perp. & (65) \end{aligned}$$

Let us prove equation (64) first.
(i) Let $|a\} \in \mathcal{I}_R$, so $\exists|b\} \in \mathcal{L}$ such that. $|a\} = \hat{A}|b\}$. Then $\forall|c\} \in \mathcal{N}_L$, $\{c|a\} = \{c|\hat{A}|b\} = 0$, and therefore $|a\} \in \mathcal{N}_L^\perp$. So, $\mathcal{I}_R \subseteq \mathcal{N}_L^\perp$.
(ii) Let $|a\} \in \mathcal{I}_R^\perp$, so $\forall|b\} \in \mathcal{L}$, $\{a|(\hat{A}|b\}) = 0$, $\{a|\hat{A} = 0$, and therefore $|a\} \in \mathcal{N}_L$ So, $\mathcal{I}_R^\perp \subseteq \mathcal{N}_L = (\mathcal{N}_L^\perp)^\perp$.
Combining (i) and (ii) with the fact that $\mathcal{A} \subseteq \mathcal{B} \iff \mathcal{A}^\perp \supseteq \mathcal{B}^\perp$ immediately gives (64). Equation (65) need not be proved separately since it changes to (64) after formal substitution of the operator under consideration $\hat{A} \to \hat{A}^\dagger$.
Let $|a\} \in \mathcal{N}_L^\perp = \mathcal{I}_R$. So, $\exists \lim_{z\to 0}(z - \hat{A})^{-1}|a\} = |c\}$ since $-\hat{A}|c\} \in \mathcal{I}_R$. Then, of course $\mathrm{Res}_{z=0}(z-\hat{A})^{-1}|a\} = 0$. Analogously for $|b\} \in \mathcal{N}_R^\perp = \mathcal{I}_L$, we have $\mathrm{Res}_{z=0}\{b|(z-\hat{A})^{-1} = 0$. The most general form of the residuum of the resolvent which remains is $\in Lin(\mathcal{N}_L, \mathcal{N}_R)$,

$$\operatorname*{Res}_{z=0}(z - \hat{A})^{-1} = \sum_{n,l=1}^{d} c_{nl}|R_n\}\{L_l|. \tag{66}$$

The unknown coefficients c_{nl} can be determined by applying (66) on $|R_{n'}\}$ and observing that $\hat{A}$ is null when restricted to $\mathcal{N}_R$, so $(z-\hat{A})^{-1}|R_{n'}\} = z^{-1}|R_{n'}\}$ and $\operatorname*{Res}_{z=0}(z-\hat{A})^{-1}|R_{n'}\} = |R_{n'}\}$. Since vectors $|R_{n'}\}$ are linearly independent, the coefficients c_{nl} satisfy

$$\sum_{n,l=1}^{d} c_{nl}\{L_l|R_{n'}\} = \delta_{nn'}, \tag{67}$$

so they are the elements of the inverse martrix (63). q.e.d.

Let us return to physics. We have shown above (see equations (58, 61)) that the operator $(1-\hat{T}_{-\sigma}(E_0,y_0)\hat{T}_\sigma(E_0,y_0))$ has left and right null-space of dimension d spanned by $|-\sigma n^*\}$ and $|\sigma n\}$, $n=1\ldots d$, respectively. Let us now try to evaluate the residuum of its inverse

$$\begin{aligned}\operatorname*{Res}_{E=E_0}\left(1-\hat{T}\right)^{-1} &= \operatorname*{Res}_{E=E_0}\left(1-\hat{T}^0-(E-E_0)\partial_E\hat{T}^0\right)^{-1} = \\ &= -\operatorname*{Res}_{z=0}\left(z-(\partial_E\hat{T}^0)^{-1}(1-\hat{T}^0)\right)^{-1}(\partial_E\hat{T}^0)^{-1} = \\ &= -\sum_{n,l=1}^{d} Inv_{nl}\left[\{-\sigma n^*|\partial_E\hat{T}^0|\sigma l\}\right]|\sigma n\}\{-\sigma l^*| = \\ &= -\sum_{n,l=1}^{d} Inv_{nl}\left[\{\uparrow n^*|\partial_E\hat{T}^0_\uparrow|\uparrow l\}+\{\downarrow n^*|\partial_E\hat{T}^0_\downarrow|\downarrow l\}\right]|\sigma n\}\{-\sigma l^*|\end{aligned}\tag{68}$$

where shorthand notation $\hat{T}=\hat{T}_{-\sigma}(E,y_0)\hat{T}_\sigma(E,y_0)$, $\hat{A}^0=\hat{A}(E_0,y_0)$ was introduced to avoid lengthy expressions. We have used lemma 2 with $\hat{A}=(\partial_E\hat{T}^0)^{-1}(1-\hat{T}^0)$, $|R_n\}=|\sigma n\}$, $\{L_n|=\{-\sigma n^*|\partial_E\hat{T}^0$, differentiated $\hat{T}^0$ as a product, and in the end used transformations (57,60).

Therefore we have to study energy derivatives of the SOS-SOS propagators $\partial_E\hat{T}_\sigma(E,y)$. In analogy with the procedure in Section III, we start by asking for y-dependence of $\hat{T}_\sigma(E,y)$ first. Take arbitrary one-side solution of the Schrödinger equation $\Psi(\boldsymbol{x},y)$, $|\Psi\rangle\in\mathcal{H}^\sigma_{Ey_1}$. By using lemma 1 we can calculate the values of the solution and its normal derivative on any SOS $\mathcal{S}_y$ for $\sigma y_1\le\sigma y\le\sigma y_\sigma$ (i.e. everywhere $y_\downarrow\le y\le y_\uparrow$ since y_1 was arbitrary)

$$\Psi(\boldsymbol{x},y) = \frac{\sqrt{-im}}{\hbar}\{\boldsymbol{x}|\hat{K}^{-1/2}(E,y)\left(1+\hat{T}_\sigma(E,y)\right)|\psi\},\tag{69}$$

$$\partial_y\Psi(\boldsymbol{x},y) = \sigma\frac{\sqrt{im}}{\hbar}\{\boldsymbol{x}|\hat{K}^{1/2}(E,y)\left(1-\hat{T}_\sigma(E,y)\right)|\psi\}.\tag{70}$$

Noting the completeness of position states $|\boldsymbol{x}\}$ one can express $|\psi\}$ from (69) and insert it to (70) and obtain very useful relation between the values and derivatives of the wavefunction on the SOS in terms of the SOS-SOS propagator $\hat{T}_\sigma$

$$\int_{\mathcal{S}} d\boldsymbol{x}\partial_y\Psi(\boldsymbol{x},y)|\boldsymbol{x}\} = i\sigma\hat{K}^{1/2}(1-\hat{T}_\sigma)(1+\hat{T}_\sigma)^{-1}\hat{K}^{1/2}\int_{\mathcal{S}} d\boldsymbol{x}\Psi(\boldsymbol{x},y)|\boldsymbol{x}\}.\tag{71}$$

Differentiate the equation (71) with respect to y and use the Schrödinger equation in a rather unusual form (which can be seen by the definition 3 of the operator $\hat{K}(E,y)$)

$$\left(\partial_y^2+\hat{K}^2(\boldsymbol{x},y)\right)\int_{\mathcal{S}} d\boldsymbol{x}\Psi(\boldsymbol{x},y)|\boldsymbol{x}\}=0\tag{72}$$

on the LHS, and apply formula (71) again on the RHS to eliminate the normal derivatives $\partial_y\Psi(\boldsymbol{x},y)$. We have used $\partial_y|\boldsymbol{x}\}_y\equiv 0$ which is compatible with the definition of the $y-$derivative of an operator-valued function which will be given in the next paragraph.

Since $\Psi(\boldsymbol{x}, y)$ is arbitrary for a given y, the vector $\int d\boldsymbol{x}\Psi(\boldsymbol{x}, y)|\boldsymbol{x}\}$ runs over entire space $\mathcal{L}_y$, so the operators in front of it on the LHS and RHS should be equal

$$-\hat{K}^2 = i\sigma\partial_y\left(\hat{K}^{1/2}(1-\hat{T}_\sigma)(1+\hat{T}_\sigma)^{-1}\hat{K}^{1/2}\right) - \hat{K}^{1/2}(1-\hat{T}_\sigma)(1+\hat{T}_\sigma)^{-1}\hat{K}(1-\hat{T}_\sigma)(1+\hat{T}_\sigma)^{-1}\hat{K}^{1/2}.$$

After formal algebraic manipulation and with the definition of few new symbols

$$[\hat{A}, \hat{B}]_\pm = \hat{A}\hat{B} \pm \hat{B}\hat{A}, \tag{73}$$

$$\hat{K}_\pm = \frac{1}{2}\left[\partial_y(\hat{K}^{1/2}), \hat{K}^{-1/2}\right]_\pm, \tag{74}$$

where $\hat{K}^{-1/2} = (\hat{K}^{1/2})^{-1}$, one obtains closed first order operator Riccati equation for the SOS-SOS propagator

$$\partial_y\hat{T}_\sigma = -i\sigma[\hat{K}, \hat{T}_\sigma]_+ + [\hat{K}_-, \hat{T}_\sigma]_- + \hat{K}_+ - \hat{T}_\sigma\hat{K}_+\hat{T}_\sigma \tag{75}$$

with the initial condition

$$\hat{T}_\sigma(E, y_\sigma) = 0 \tag{76}$$

assuming that on the boundary $y = y_\sigma$ all SOS-wavenumbers $k_n(E, y_\sigma)$ are imaginary. (If not, they can be made such if the (fictitious) hard walls on the boundaries $y = y_\sigma$, which ensure the Dirichlet boundary conditions, are infinitesimally smoothed.)

A remark is in order concerning the derivation in the last paragraph: The derivative of the propagator $\hat{T}_\sigma(E, y)$ with respect to y is perfectly well defined, although $\hat{T}_\sigma(E, y)$ and $\hat{T}_\sigma(E, y + dy)$ act in different Hilbert spaces, since the latter are isomorphic. So for any such operator-valued function of y $\hat{A}(y) \in Lin(\mathcal{L}_y)$, one should define

$$\partial_y\hat{A}(y) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left(\hat{I}_{y,y+\epsilon}\hat{A}(y+\epsilon)\hat{I}_{y+\epsilon,y} - \hat{A}(y)\right). \tag{77}$$

We shall also need the y-derivatives of the SOS-CS-SOS propagators $\partial_y\hat{Q}_\sigma(E, y)$ and $\partial_y\hat{P}_\sigma(E, y)$. Let us start by calculating the values of $\partial_y\hat{Q}_\sigma(E, y)|\psi\}$ on the SOS $\mathcal{S}_y$ for any $|\psi\} \in \mathcal{L}_y$.

$$\begin{aligned}
\langle\boldsymbol{x}, y'|\partial_y\hat{Q}_\sigma(E, y)|\psi\}|_{\sigma y'\searrow\sigma y} &= \partial_y\left(\langle\boldsymbol{x}, y|\hat{Q}_\sigma(E, y)|\psi\}\right) - \partial_{y'}\langle\boldsymbol{x}, y'|\hat{Q}_\sigma(E, y)|\psi\}|_{\sigma y'\searrow\sigma y} = \\
&= \frac{\sqrt{im}}{\hbar}\{\boldsymbol{x}|\left[\partial_y\left(\hat{K}^{-1/2}(1+\hat{T}_\sigma)\right) - i\sigma K^{1/2}(1-\hat{T}_\sigma)\right]|\psi\} = \\
&= \langle\boldsymbol{x}, y|\hat{Q}_\sigma\left[-i\sigma\hat{K} - \hat{K}_- - \hat{K}_+\hat{T}_\sigma\right]|\psi\},
\end{aligned} \tag{78}$$

where the equations (19,54) and (75) and some operator algebra were applied. Note that the derivative of the solution of the Schrödinger equation $\Psi(\boldsymbol{x}, y') = \langle\boldsymbol{x}, y'|\hat{Q}_\sigma(E, y)|\psi\}$ with respect to smooth external parameter y is again solution of the Schrödinger equation, $\partial_y\hat{Q}_\sigma(E, y)|\psi\} \in \mathcal{H}^\sigma_{Ey}$. The solution of the *linear* Schrödinger equation is a unique and *linear* function of boundary conditions, so the linear relation for boundary condition (78) holds also globally (and since ket $|\psi\}$ is arbitrary it can be omitted)

$$\partial_y\hat{Q}_\sigma = \hat{Q}_\sigma\left[-i\sigma\hat{K} - \hat{K}_- - \hat{K}_+\hat{T}_\sigma\right]. \tag{79}$$

One can completely analogously derive similar equation for another propagator $\hat{P}_\sigma(E, y)$

$$\partial_y\hat{P}_\sigma = \left[-i\sigma\hat{K} + \hat{K}_- - \hat{T}_\sigma\hat{K}_+\right]\hat{P}_\sigma. \tag{80}$$

In analogy with 1-dimensional case (although this definition slightly differs from that in Section III) we define also an *incomplete normalization operator* $\hat{N}_\sigma(E,y) \in Lin(\mathcal{L}_y)$,

$$\hat{N}_\sigma(E,y) = \sigma \int_{\mathcal{S}} d\boldsymbol{x} \int_y^{y_\sigma} dy' \hat{P}_\sigma(E,y)|\boldsymbol{x},y'\rangle\langle\boldsymbol{x},y'|\hat{Q}_\sigma(E,y) = \tag{81}$$

$$= \hat{P}_\sigma(E,y)\hat{Q}_\sigma(E,y). \tag{82}$$

We are again interested in the derivative of the incomplete normalization operator with respect to y. So far we have ignored the discontinuities of $\langle\boldsymbol{x},y'|\hat{Q}_\sigma(E,y)$ and $\hat{P}_\sigma(E,y)|\boldsymbol{x},y'\rangle$ at $y'=y$ by always approaching $y' \to y$ from the proper side, so we have to take representation (81) to account for the discontinuities, and calculate

$$\begin{aligned}\partial_y \hat{N}_\sigma(E,y) &= \left(\partial_y \hat{P}_\sigma(E,y)\right)\hat{Q}_\sigma(E,y) + \hat{P}_\sigma(E,y)\partial_y\hat{Q}_\sigma(E,y) - \\ &- \sigma \int_{\mathcal{S}} d\boldsymbol{x} \hat{P}_\sigma(E,y)|\boldsymbol{x},y\rangle\langle\boldsymbol{x},y|\hat{Q}_\sigma(E,y).\end{aligned}$$

The remaining integral over the SOS can be calculated by means of initial data (19,20)

$$\int_{\mathcal{S}} d\boldsymbol{x} \hat{P}_\sigma(E,y)|\boldsymbol{x},y\rangle\langle\boldsymbol{x},y|\hat{Q}_\sigma(E,y) = -\frac{im}{\hbar^2}(1+\hat{T}_\sigma)\hat{K}^{-1}(1+\hat{T}_\sigma),$$

so after applying formulas (79,80) one can write the differential system for the incomplete normalization operator

$$\begin{aligned}\partial_y \hat{N}_\sigma &= -i\sigma[\hat{K},\hat{N}_\sigma]_+ + [\hat{K}_-,\hat{N}_\sigma]_- - \hat{T}_\sigma\hat{K}_+\hat{N}_\sigma - \hat{N}_\sigma\hat{K}_+\hat{T}_\sigma + \\ &+ i\sigma\frac{m}{\hbar^2}(1+\hat{T}_\sigma)\hat{K}^{-1}(1+\hat{T}_\sigma),\end{aligned} \tag{83}$$

$$\hat{N}_\sigma(E,y_\sigma) = 0, \tag{84}$$

which is linear in $\hat{N}_\sigma$, but depends again quadratically on $\hat{T}_\sigma$ (compare with (75)). Now we have the tools to ask for the derivative of the SOS-SOS propagator with respect to the energy $\partial_E\hat{T}_\sigma$. It can be determined as a unique solution of the first-order differential system

$$\partial_y\left(\partial_E\hat{T}_\sigma\right) = \partial_E\left(\partial_y\hat{T}_\sigma\right), \tag{85}$$

$$\partial_E\hat{T}_\sigma(E,y_\sigma) = 0, \tag{86}$$

which is the obvious requirement for the uniqueness of the mixed second derivative. The initial condition (86) is just an energy derivative of the initial condition (76). The author has guessed the solution in analogy with 1-dimensional case (Section III)

$$\partial_E\hat{T}_\sigma = -\hat{N}_\sigma + \frac{m}{2\hbar^2}\left(\hat{K}^{-2} - \hat{T}_\sigma\hat{K}^{-2}\hat{T}_\sigma\right). \tag{87}$$

The reader can verify the consistency of (87) by inserting it into (85) and applying the formulas (75,83) and the formulas

$$\partial_E\hat{K}^p = \frac{m}{\hbar^2}p\hat{K}^{p-2}, \tag{88}$$

$$\partial_E\hat{K}_- = \frac{m}{2\hbar^2}[\hat{K}^{-2},\hat{K}_+]_-, \tag{89}$$

$$\partial_E\hat{K}_+ = \frac{m}{2\hbar^2}\left([\hat{K}^{-2},\hat{K}_-]_- + \partial_y(\hat{K}^{-2})\right), \tag{90}$$

which can be derived directly from the definitions and with a bit of operator algebra, of course.

Now we can finish the calculation of the residuum (68). First we use our new result (87) and the formulae (57,60) and (52,59) with definition (81) to calculate the matrix elements

$$\begin{aligned}\{\uparrow n^*|\partial_E \hat{T}^0_\uparrow|\uparrow l\} + \{\downarrow n^*|\partial_E \hat{T}^0_\downarrow|\downarrow l\} &= -\{\uparrow n^*|\hat{N}^0_\uparrow|\uparrow l\} - \{\downarrow n^*|\hat{N}^0_\downarrow|\downarrow l\} = \\ &= -\int_{\mathcal{S}} d\boldsymbol{x} \left(\int_y^{y_\uparrow} dy' + \int_{y_\downarrow}^{y} dy' \right) \Psi_n^*(\boldsymbol{x}, y')\Psi_l(\boldsymbol{x}, y') = \\ &= -\delta_{nl},\end{aligned}$$

since the eigenstates $|\Psi_n\rangle$ are supposed to be orthonormal $\langle\Psi_n|\Psi_l\rangle = \delta_{nl}$. The residuum (68) is therefore very simple

$$\operatorname*{Res}_{E=E_0} (1-\hat{T})^{-1} = \sum_{n=1}^{d} |\sigma n\}\{-\sigma n^*|. \tag{91}$$

The calculation of the residuum of the general Green's function (21) is now straightforward

$$\begin{aligned}\operatorname*{Res}_{E=E_0} \langle \boldsymbol{q}'|\hat{G}(E)|\boldsymbol{q}\rangle &= \sum_{\sigma,n} \langle \boldsymbol{q}'|\hat{Q}^0_\sigma|\sigma n\}\{-\sigma n^*|\hat{P}^0_{-\sigma}|\boldsymbol{q}\rangle + \\ &+ \sum_{\sigma,n} \langle \boldsymbol{q}'|\hat{Q}^0_\sigma|\sigma n\}\{-\sigma n^*|\hat{T}^0_{-\sigma}\hat{P}^0_\sigma|\boldsymbol{q}\rangle = \\ &= \sum_{\sigma,\sigma',n} \langle \boldsymbol{q}'|\hat{Q}^0_{\sigma'}|\sigma' n\}\{\sigma n^*|\hat{P}^0_\sigma|\boldsymbol{q}\rangle = \\ &= \sum_n \Psi_n(\boldsymbol{q}')\Psi_n^*(\boldsymbol{q}).\end{aligned} \tag{92}$$

This completes the proof of the general decomposition formula.

V. DISCUSSION AND CONCLUSIONS

In this paper I have presented and proved the decomposition of the resolvent $\hat{G}(E) = (E-\hat{H})^{-1}$ (formula (21)) in terms of four newly defined energy-dependent propagators from and/or to Hilbert space of complex-valued functions over f-dim configuration space (CS) (kets and bras with angle brackets) to and/or from Hilbert space of complex-valued functions over $(f-1)$-dim configurational surface of section (SOS) (kets and bras with curly brackets) which have the following clear physical interpretations

- $\langle \boldsymbol{q}'|\hat{G}_0(E,y)|\boldsymbol{q}\rangle$ is a quantum probability amplitude that the system propagates from point $\boldsymbol{q}$ to point $\boldsymbol{q}'$ at energy E without hitting the SOS labeled by y.
- $\{\boldsymbol{x}|\hat{P}_\sigma(E,y)|\boldsymbol{q}\rangle$ is a probability amplitude that the system propagates from point $\boldsymbol{q}$ above (if $\sigma=\uparrow$) or below (if $\sigma=\downarrow$) SOS to the point $\boldsymbol{x}$ on the SOS at energy E and without hitting the SOS in between.
- $\langle \boldsymbol{q}|\hat{Q}_\sigma(E,y)|\boldsymbol{x}\}$ is a probability amplitude that the system propagates from point $\boldsymbol{x}$ on the SOS to the point $\boldsymbol{q}$ in the CS above (if $\sigma=\uparrow$) or below (if $\sigma=\downarrow$) SOS at energy E without hitting the SOS in between.

- $\{\boldsymbol{x}'|\hat{T}_\sigma(E,y)|\boldsymbol{x}\}$ is a probability amplitude that the system propagates from point $\boldsymbol{x}$ on the SOS to the point $\boldsymbol{x}'$ on the SOS through the upper (if $\sigma =\uparrow$) or lower (if $\sigma =\downarrow$) part of CS with respect to the SOS and at energy E without hitting the SOS in between.

All these propagators are analytic (holomorphic) in the upper half energy plane, $\mathrm{Im}E > 0$. By expressing them in terms of the resolvent of the related scattering Hamiltonian [7] one can show that they can have typically a *finite number of poles* on the *real energy-axis* or they have even no poles on the entire real energy-axis if a given SOS $\mathcal{S}_y$ is being crossed by every classical trajectory, heuristically speaking (or the corresponding scattering problem, whoose S-matrix is just our propagator $\hat{T}_\sigma(E,y)$ [7], has no bound states, rigorously speaking).

Using this interpretation one can arrive at the decomposition formula (in expanded form (22)) heuristically, just by using basic postulates of quantum mechanics about addition and multiplication of probability amplitudes and knowing that typical quantum path is continuous (but not differentiable) [3] (this is why the signs $\uparrow$ and $\downarrow$ are alternating in the decomposition formula (22).)

In case where there is a time-reversal symmetry, the quantum Poincaré (SOS-SOS) map is symmetric in position representation [8, 10]

$$\{\boldsymbol{x}'|\hat{T}_\sigma|\boldsymbol{x}\} = \{\boldsymbol{x}|\hat{T}_\sigma|\boldsymbol{x}'\}. \tag{93}$$

It can also be shown [8, 10] that if the SOS-SOS operator is represented by a finite-dimensional matrix $T^\sigma_{n'n} = \{n'|\hat{T}_\sigma|n\}$ in a truncated basis $\{|n\}; k_n^2 > 0\}$ where we discard all evanescent (closed) SOS-eigenmodes with imaginary wavenumbers then the matrix $T^\sigma_{n'n}$ is unitary.

The quantum surface of section is expected to be of great practical (numerical) value since the dimension of the truncated matrices of the SOS-SOS propagators (which is $\mathcal{O}\left(\hbar^{1-f}\right)$) can be orders of magnitude smaller than the dimension of the truncated matrix of the full Hamiltonian (which is $\mathcal{O}\left(\hbar^{-f}\right)$). Thus the practical algorithms based on quantum SOS method for calculation of energy spectra can be developed which are orders of magnitude faster than the existing ones.

The determination of the exact SOS-SOS propagator (unlike the semiclassical one as in [1]) is still quite a difficult task. Solving the Riccati equations (39,75) of the propagator flow through the family of surfaces of section is quite elaborate, even numerically. One would wish to have a direct method which has been so far successful only for special systems, like free particle on a "trombone" attached to a parallelogram[4], or Sinai billiard[11]. The author succeeded to find explicit procedure for calculation of the SOS-SOS propagator for the so-called *semi-separable systems*, which are separable for $y > y_0$, and for $y < y_0$, but they are possibly discontinuous at $y = y_0$. The method has already been applied to one such 2-dim system with generic nonintegrable classical dynamics [9] and energy levels with sequential quantum number around 20 million were easily calculated (1 - 3 minutes of supercomputer (Convex C3860) CPU time per level).

Some of the open problems of the subject are: (i) developing the phase-space version of the present theory e.g. in the Wigner-Weyl language, (ii) developing practical methods for evaluating exact SOS-propagators in concrete examples, (iii) establishing the connection between the present formalism and path integrals with geometrical constraints which are still to be defined for this purpose, whereas (iv) generalization of the present theory, e.g.

to cases of general magnetic fields where the component of the momentum perpendicular to SOS does no longer enter the Hamiltonian only quadratically but also linearly, and (v) study of the semiclassical limit were already acomplished in [8].

In the present theory the algebra of the generators of parallel motions (with respect to the SOS) need not be just the operator algebra spanned by $(\boldsymbol{x}, \boldsymbol{p}_x)$. Indeed an obvious generalization is possible by considering an arbitrary Lie algebra instead, since we always refer just to inside Hamiltonian $\hat{H}'$ (see equation (3)) as a whole and never to $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{p}}_x$ separately. For example, instead of ordinary position and momentum, $\boldsymbol{x}$ and $\boldsymbol{p}_x$, we could have angular momentum or spin coordinates J_1, J_2, J_3.

ACKNOWLEDGMENTS

I am grateful to Professor Marko Robnik for proposing the semiclassical version of this project which lead me to the present work, for the discussions on the subject, and for reading the manuscript. The financial support by the Ministry of Science and Technology of the Republic of Slovenia is gratefully acknowledged.

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Figure captions

Figure 1 Illustration of one of the terms in the expanded form of the decomposition formula for the energy dependent propagator (22), namely $\hat{Q}_\downarrow \hat{T}_\uparrow \hat{T}_\downarrow \hat{P}_\uparrow$. A typical continuous (but nondifferentiable) path which contributes to this term is shown and the corresponding probability amplitudes are marked. The latter have to be multiplied and sumed (integrated) over the intersection points $\boldsymbol{x}, \boldsymbol{x}'$ and $\boldsymbol{x}''$ in order to yield the probability amplitude for the entire term, namely the probability amplitude to propagate from point $\boldsymbol{q}$ to point $\boldsymbol{q}'$ at definite energy E and crossing the SOS exactly three times $\langle \boldsymbol{q}' | \hat{Q}_\downarrow \hat{T}_\uparrow \hat{T}_\downarrow \hat{P}_\uparrow | \boldsymbol{q} \rangle$.